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=> s mass (w) spectrometry and peptide(w)ladder
L1 73 MASS (W) SPECTROMETRY AND PEPTIDE(W) LADDER

=> d 65-70 abs

L1 ANSWER 65 OF 73 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN

AB Advances in proteomics are continuing to expand the ability to analyze the serum proteome. In recent years, it has been realized that in addition to the circulating proteins, human serum also contains a large number of peptides. Many of these peptides are believed to be fragments of larger proteins that have been at least partially degraded by various enzymes such as metalloproteases. Identifying these peptides from a small amount of serum/plasma is difficult due to the complexity of the sample, the low levels of these peptides, and the difficulties in getting a protein identification from a single peptide. In this study, we modified previously published protocols for using centrifugal ultrafiltration, and unlike past studies did not digest the filtrate with trypsin with the intent of identifying endogenous peptides with this method. The filtrate fraction was concentrated and analyzed by a reversed phase-high performance liquid chromatography system connected to a nanospray ionization hybrid ion trap-Fourier transform mass spectrometer (LTQ-FTMS). The mass accuracy of this instrument allows confidence for identifying the protein precursors by a single peptide. The utility of this approach was demonstrated by the identification of over 300 unique peptides with 2 ppm or better mass accuracy per serum sample. With confident identifications, the origin and function of native serum peptides can be more seriously explored. Interestingly, over 34 **peptide ladders** were observed from over 17 serum proteins. This indicates that a cascade of proteolytic processes affects the serum peptidome. To examine whether this result was an artifact of serum, matched plasma and serum samples were analyzed with similar **peptide ladders** found in each. .COPYRG. 2006 Elsevier B.V. All rights reserved.

L1 ANSWER 66 OF 73 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN

AB A method for the rapid identification of high-affinity ligands to Src homology-2 (SH2) domains is reported. A phosphotyrosyl (pY) peptide library containing completely randomized residues at positions -2 to +3 relative to the pY was synthesized on Tentagel resin, with a unique peptide sequence on each resin bead (total 2.5×10^6 different sequences). The library was screened against the biotinylated N- and C-terminal SH2

domains of protein tyrosine phosphatase SHP-1, and the beads that carry high-affinity ligands of the SH2 domains were identified using an enzyme-linked assay involving a streptavidin-alkaline phosphatase conjugate. **Peptide ladder** sequencing of the selected beads using matrix-assisted laser desorption ionization **mass spectrometry** revealed consensus sequences for both SH2 domains. The N-terminal SH2 domain strongly selects for peptides with a leucine at the -2 position; at the C-terminal side of the pY residue, it can recognize two distinct classes of peptides with consensus sequences of LXpY(M/F)X(F/M) and LXpYAXL (X = any amino acid), respectively. The C-terminal SH2 domain exhibits almost exclusive selectivity for peptides of the consensus sequence, (V/I/L)XpYAX(L/V). Several representative sequences selected from the library were individually synthesized and tested for binding to the SH2 domains by surface plasmon resonance and for their ability to stimulate the catalytic activity of SHP-1. Both experiments have demonstrated that the selected peptides are capable of binding to the SH2 domains with dissociation constants (K(D)) in the low micromolar range.

- L1 ANSWER 67 OF 73 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
- AB Biopolymer sequencing with **mass spectrometry** has become increasingly important and accessible with the development of matrix-assisted laser desorption/ionization (MALDI) and electrospray ionization (ESI). Here we examine the use of sequential digestion for the rapid identification of proteolytic fragments, in turn highlighting the general utility of enzymatic MALDI ladder sequencing and ESI tandem **mass spectrometry**. Analyses were performed on oligonucleotides ranging in size from 2 to 50 residues, on peptides ranging in size from 7 to 44 residues and on viral coat proteins. MALDI ladder sequencing using exonuclease digestion generated a uniform distribution of ions and provided complete sequence information on the oligonucleotides 2-30 nucleic acid residues long. Only partial sequence information was obtained on the longer oligonucleotides. C-terminal **peptide ladder** sequencing typically provided information from 4 to 7 amino acids into the peptide. Sequential digestion, or endoprotease followed by exoprotease exposure, was also successfully applied to a trypsin digest of viral proteins. Analysis of ladder sequenced peptides by LCMS generated less information than in the MALDI-MS analysis and ESI-MS2 normally provided partial sequence information on both the small oligonucleotides and peptides. In general, MALDI ladder sequencing offered information on a broader mass range of biopolymers than ESI-MS2 and was relatively straightforward to interpret, especially for oligonucleotides. Copyright (C) 1998 Elsevier Science Ltd.
- L1 ANSWER 68 OF 73 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
- AB The techniques of enzymatic and chemical **peptide ladder** sequencing, coupled with ultraviolet - matrix assisted laser desorption/ionization - **mass spectrometry** (UV-MALDI-MS) have been improving continuously in the last five years and have now become important tools for primary structure identification. In this work, signal suppression effects, appearing in UV- MALDI-MS (excitation 337 nm) of ladder peptides, were investigated using the 17-amino acid peptide dynorphin A. We show, with examples of simple 'two-peptide' systems and more complex 'multi-peptide' systems, that suppression effects do in fact exist. The magnitude of the observed suppression is strongly dependent upon both the nature and the amount of the suppressing peptide. Suppression behavior of individual ladder peptides was investigated on equimolar mixtures of ten ladder peptides. Significant signal suppression was recorded for all ladder peptides, with some of them being approximately 170 times lower in signal intensity than the pure, i.e., unsuppressed peptide at the same concentration. For the investigated system - dynorphin A, 4- hydroxy- α -cyanocinnamic acid

(4-HCCA) matrix, UV excitation - a correlation between the extent of suppression and an intractable combination of peptide hydrophobicity and the presence of several basic amino acids can be seen.

L1 ANSWER 69 OF 73 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
AB A new modification of the **peptide ladder** sequencing technique is described in which allyl isothiocyanate (AITC) replaces trifluoroethyl isothiocyanate as the volatile amine-modification reagent. AITC is commercially available, readily purified, stable up to 80 °C and reacts cleanly and rapidly with all amino groups of polypeptides. Several model peptides and two side chain-modified peptides were sequentially degraded using AITC and the cleavage reagent heptatluorobutyric acid (HFBA) up to seven amino acids from the N-terminus. Matrix-assisted laser-desorption and ionization coupled with time-of-flight (MALDI-TOF) mass spectroscopy of the peptide mixture provided a clear ladder-like mass profile with consecutive molecular ions corresponding to each shortened peptide at picomole range. The results indicate the general utility of this analytical protocol by the use of AITC as the amine-coupling reagent.

L1 ANSWER 70 OF 73 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
AB Mutation-induced amino acid exchanges occurring on the large T9 peptide of the α -chain of human hemoglobin (residues 62-90) are difficult to identify. Despite their high m/z value (around m/z 3000), collision-induced dissociation spectra of liquid secondary ion mass spectrometrically generated protonated α T9 peptides were performed successfully. In parallel electrospray **mass spectrometry** (MS) was used both to measure the molecular mass of the intact proteins and to determine the number of protonatable sites in the α T9 peptides. **Peptide ladder** sequencing using carboxypeptidase digestions and analysis of the truncated peptides by matrix-assisted laser desorption ionization time-of-flight MS confirmed the interpretation. This set of methods allowed the characterization of three hemoglobin variants, with amino acid exchanges located in the α T9 part of the sequence. Two of them, Hb Aztec [α 76(EF5) Met \rightarrow Thr] and Hb M-Iwate [α 87(F8) His \rightarrow Tyr] were already known. The third [α 89(FG1) His \rightarrow Tyr] was novel and named Hb Villeurbanne.

=> d 70 all

L1 ANSWER 70 OF 73 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
AN 97237609 EMBASE
DN 1997237609
TI Combined mass spectrometric methods for the characterization of human hemoglobin variants localized within α T9 peptide: Identification of Hb villeurbanne α 89 (FG1) His \rightarrow Tyr.
AU Deon C.; Prome J.C.; Francina A.; Groff P.; Kalmes G.; Galacteros F.; Wajcman H.
CS J.C. Prome, Institut Pharmacologie, CNRS, 205 Route de Narbonne, 31077 Toulouse Cedex, France
SO Journal of Mass Spectrometry, (1997) Vol. 32, No. 8, pp. 880-887. .
Refs: 19
ISSN: 1076-5174 CODEN: JMSPFJ
CY United Kingdom
DT Journal; Article
FS 022 Human Genetics
025 Hematology
029 Clinical Biochemistry
LA English

SL English
ED Entered STN: 22 Aug 1997
Last Updated on STN: 22 Aug 1997
AB Mutation-induced amino acid exchanges occurring on the large T9 peptide of the α -chain of human hemoglobin (residues 62-90) are difficult to identify. Despite their high m/z value (around m/z 3000), collision-induced dissociation spectra of liquid secondary ion mass spectrometrically generated protonated α T9 peptides were performed successfully. In parallel electrospray *mass spectrometry* (MS) was used both to measure the molecular mass of the intact proteins and to determine the number of protonatable sites in the α T9 peptides. *Peptide ladder* sequencing using carboxypeptidase digestions and analysis of the truncated peptides by matrix-assisted laser desorption ionization time-of-flight MS confirmed the interpretation. This set of methods allowed the characterization of three hemoglobin variants, with amino acid exchanges located in the α T9 part of the sequence. Two of them, Hb Aztec [α 76(EF5) Met \rightarrow Thr] and Hb M-Iwate [α 87(F8) His \rightarrow Tyr] were already known. The third [α 89(FG1) His \rightarrow Tyr] was novel and named Hb Villeurbanne.
CT Medical Descriptors:
*peptide analysis
article
controlled study
human
human tissue
molecular weight
mutation
priority journal
tandem mass spectrometry
technique
Drug Descriptors:
*hemoglobin variant: AN, drug analysis
*hemoglobin variant: EC, endogenous compound

=> d 73 all

L1 ANSWER 73 OF 73 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
AN 95000448 EMBASE
DN 1995000448
TI MALDI-MS for C-terminal sequence determination of peptides and proteins degraded by carboxypeptidase Y and P.
AU Thiede B.; Wittmann-Liebold B.; Bienert M.; Krause E.
CS Forschungsinst.Molekulare Pharmakol., Alfred-Kowalke-Strasse 4,D-10315 Berlin, Germany
SO FEBS Letters, (1995) Vol. 357, No. 1, pp. 65-69. .
ISSN: 0014-5793 CODEN: FEBLAL
CY Netherlands
DT Journal; Article
FS 029 Clinical Biochemistry
LA English
SL English
ED Entered STN: 25 Jan 1995
Last Updated on STN: 25 Jan 1995
AB Matrix-assisted laser desorption/ionization *mass spectrometry* (MALDI-MS) has been used for C-terminal amino acid sequence determination of peptides and proteins. The usefulness of MALDI-MS was demonstrated by analyzing peptide mixtures (C-terminal *peptide ladder*) which were generated by enzymatic digestion of substance P, glucagon, angiotensinogen, insulin B chain and myoglobin with the exopeptidases carboxypeptidase Y and P. The results clearly show that up to 11 amino acid residues can be determined in the

pmol range by analyzing the molecular masses of the truncated peptides.
For proteins it is possible to investigate enzymatic or chemical digests
in the same manner.

CT Medical Descriptors:

- *mass spectrometry*
- *protein structure
- amino acid sequence
- article
- priority journal

Drug Descriptors:

- *proline carboxypeptidase
- *serine carboxypeptidase

RN (proline carboxypeptidase) 9075-64-3; (serine carboxypeptidase) 11104-54-4

=> s merrifield (W) synthesis and PITC and PIC
L1 0 MERRIFIELD (W) SYNTHESIS AND PITC AND PIC

=> s merrifield (W) synthesis and PITC
L2 0 MERRIFIELD (W) SYNTHESIS AND PITC

=> s merrifield (W) synthesis
L3 2983 MERRIFIELD (W) SYNTHESIS

=> l3 and phenyl (w) isocyanate
L3 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s l3 and phenyl (w) isocyanate
L4 4 L3 AND PHENYL (W) ISOCYANATE

=> d all

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:539648 CAPLUS
DN 125:301535
ED Entered STN: 10 Sep 1996
TI The synthesis of 2-oxopiperazines by intramolecular Michael addition on
solid support
AU Goff, Dane A.; Zuckermann, Ronald N.
CS Chiron Corp, Emeryville, CA, 94608, USA
SO Tetrahedron Letters (1996), 37(35), 6247-6250
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 28
OS CASREACT 125:301535
AB Attempted cyclopropanation of unsatd. peptoids on solid support led to the
discovery of a facile method for generating libraries of constrained
cyclic peptoids.
ST piperazinone peptoid prepn; Michael addn intramol unsatd peptoid
IT **Merrifield synthesis**
(synthesis of oxopiperazines by intramol. Michael addition on solid
support)
IT Michael reaction
(intramol., synthesis of oxopiperazines by intramol. Michael addition on
solid support)
IT 64-04-0, Phenethylamine 78-81-9, Isobutylamine 79-08-3, Bromoacetic
acid 100-46-9, Benzylamine, reactions 103-71-9, **Phenyl**
isocyanate, reactions 495-69-2D, n-Benzoylglycine, resin-bound
5367-24-8, Dimethyloxosulfonium methylide 20629-35-0 29022-11-5, Fmoc
gly oh 35661-39-3 35661-40-6 35737-15-6, Fmoc trp oh 68858-20-8
71989-31-6 182552-58-5D, resin-bound 182552-61-0D, resin-bound
182552-63-2D, resin-bound
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of oxopiperazines by intramol. Michael addition on solid
support)
IT 182552-51-8DP, resin-bound 182552-52-9DP, resin-bound 182552-59-6DP,
resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Préparation); RACT
(Reactant or reagent)
(synthesis of oxopiperazines by intramol. Michael addition on solid
support)
IT 182552-53-0P 182552-54-1P 182552-55-2P 182552-56-3P 182552-57-4P

182552-60-9P 182552-62-1P 182552-64-3P 182820-67-3P 182820-68-4P
182820-69-5P 182820-70-8P 182820-71-9P 182820-72-0P 182820-73-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of oxopiperazines by intramol. Michael addition on solid support)

=> d 1-4 all

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:539648 CAPLUS
DN 125:301535
ED Entered STN: 10 Sep 1996
TI The synthesis of 2-oxopiperazines by intramolecular Michael addition on solid support
AU Goff, Dane A.; Zuckermann, Ronald N.
CS Chiron Corp, Emeryville, CA, 94608, USA
SO Tetrahedron Letters (1996), 37(35), 6247-6250
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 28
OS CASREACT 125:301535
AB Attempted cyclopropanation of unsatd. peptoids on solid support led to the discovery of a facile method for generating libraries of constrained cyclic peptoids.
ST piperazinone peptoid prepn; Michael addn intramol unsatd peptoid
IT **Merrifield synthesis**
(synthesis of oxopiperazines by intramol. Michael addition on solid support)
IT Michael reaction
(intramol., synthesis of oxopiperazines by intramol. Michael addition on solid support)
IT 64-04-0, Phenethylamine 78-81-9, Isobutylamine 79-08-3, Bromoacetic acid 100-46-9, Benzylamine, reactions 103-71-9, **Phenyl isocyanate**, reactions 495-69-2D, n-Benzoylglycine, resin-bound 5367-24-8, Dimethyloxosulfonium methylide 20629-35-0 29022-11-5, Fmoc gly oh 35661-39-3 35661-40-6 35737-15-6, Fmoc trp oh 68858-20-8 71989-31-6 182552-58-5D, resin-bound 182552-61-0D, resin-bound 182552-63-2D, resin-bound
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of oxopiperazines by intramol. Michael addition on solid support)
IT 182552-51-8DP, resin-bound 182552-52-9DP, resin-bound 182552-59-6DP, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of oxopiperazines by intramol. Michael addition on solid support)
IT 182552-53-0P 182552-54-1P 182552-55-2P 182552-56-3P 182552-57-4P
182552-60-9P 182552-62-1P 182552-64-3P 182820-67-3P 182820-68-4P
182820-69-5P 182820-70-8P 182820-71-9P 182820-72-0P 182820-73-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of oxopiperazines by intramol. Michael addition on solid support)

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:457334 CAPLUS
DN 125:221769
ED Entered STN: 02 Aug 1996
TI Solid-phase synthesis of 5,6-dihydropyrimidine-2,4-diones
AU Kolodziej, Stephen A.; Hamper, Bruce C.

CS Ceregen Div. Monsanto Corporation, St. Louis, MO, 63167, USA
 SO Tetrahedron Letters (1996), 37(30), 5277-5280
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier
 DT Journal
 LA English
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
 AB A series of 1,3-disubstituted-5,6-dihydropyrimidine-2,4-diones (1) are prepared by solid phase organic chemical using a cyclization-cleavage strategy from readily available amines and isocyanates. An acrylate ester of Wangs resin is treated with primary amines to afford N-substituted β -aminoesters followed by treatment with isocyanates to afford β -ureido ester. Cyclization-cleavage of the bound ureido ester under acidic conditions gave direct formation of 5,6-dihydropyrimidinedione 1.
 ST pyrimidinedione hydro solid phase prepn
 IT **Merrifield synthesis**
 (solid-phase synthesis of 5,6-dihydropyrimidine-2,4-diones)
 IT 5426-62-ODP, polymer bound 21575-64-4P 75873-79-9P 181463-48-9P
 181463-50-3P 181463-52-5P 181463-57-0P 181463-60-5P 181463-64-9P
 181463-69-4P 181463-72-9P 181463-74-1P 181463-76-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 64-04-0, Phenethylamine 74-89-5, Methylamine, reactions 75-31-0,
 Isopropylamine, reactions 78-81-9, Isobutylamine 100-46-9,
 Benzylamine, reactions 103-71-9, **Phenyl isocyanate**,
 reactions 107-11-9, Allylamine 614-68-6, o-Tolyl isocyanate
 624-83-9, Methyl isocyanate 814-68-6, Acryloyl chloride 924-73-2,
 β -Alanine ethyl ester 1795-48-8, Isopropyl isocyanate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (solid-phase synthesis of 5,6-dihydropyrimidine-2,4-diones)
 IT 33351-38-1DP, polymer bound 181463-78-5DP, polymer bound
 181463-82-1DP, polymer bound 181463-86-5DP, polymer bound
 181463-92-3DP, polymer bound 181464-02-8DP, polymer bound
 181464-08-4DP, polymer bound 181464-14-2DP, polymer bound
 181464-20-ODP, polymer bound 181464-25-5DP, polymer bound
 181464-33-5DP, polymer bound 181464-40-4DP, polymer bound
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (solid-phase synthesis of 5,6-dihydropyrimidine-2,4-diones)
 L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1996:397488 CAPLUS
 DN 125:167902
 ED Entered STN: 11 Jul 1996
 TI Solid-phase synthesis of 1,3-dialkylquinazoline-2,4-diones
 AU Buckman, Brad O.; Mohan, Raju
 CS New Lead Discovery, Berlex Biosci., Richmond, CA, 94804-0099, USA
 SO Tetrahedron Letters (1996), 37(26), 4439-4442
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier
 DT Journal
 LA English
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
 OS CASREACT 125:167902
 AB A library of 1,3-dialkyl-6-hydroxyquinazoline-2,4-diones (9) has been synthesized on a polymeric support by a three step approach. Addition of isocyanates or amines to a polymer-supported anthranilate derivative affords ureas which can be cyclized to 3-alkylquinazolinediones. N-Alkylation at the 1-position and cleavage from the resin affords 9 in high yield and purity.
 ST quinazolinedione dialkyl solid phase synthesis; solid phase synthesis
 dialkylquinazolinedione; anthranilate polymer supported reaction
 isocyanate
 IT **Merrifield synthesis**

(solid-phase synthesis of dialkylquinazolinediones)

IT 75-03-6, Ethyl iodide 86-84-0, 1-Naphthyl isocyanate 100-28-7,
p-Nitrophenyl isocyanate 100-39-0, Benzyl bromide 103-71-9,
Phenyl isocyanate, reactions 106-95-6, Allyl bromide,
reactions 107-08-4, Propyl iodide 123-00-2, 4-Morpholinepropanamine
462-08-8, 3-Pyridinamine 541-28-6, 3-Methylbutyl iodide 614-68-6,
o-Tolyl isocyanate 624-83-9, Methyl isocyanate 1195-45-5,
p-Fluorophenyl isocyanate 1476-23-9, Allyl isocyanate 1882-72-0
3173-56-6, Benzyl isocyanate 3433-80-5, o-Bromobenzyl bromide
4392-24-9, Cinnamyl bromide 5036-48-6, 1h-Imidazole-1-propanamine
5416-93-3, p-Anisyl isocyanate 6628-04-2 7693-46-1, p-Nitrophenyl
chloroformate 16588-74-2, 3,5-Bis(trifluoromethyl)**phenyl**
isocyanate 91913-67-6 155505-56-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(solid-phase synthesis of dialkylquinazolinediones)

IT 1882-72-0DP, polymer-bound 180297-14-7P 180297-15-8P 180297-16-9DP,
polymer-bound 180297-17-0DP, polymer-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(solid-phase synthesis of dialkylquinazolinediones)

IT 180296-99-5P 180297-00-1P 180297-01-2P 180297-02-3P 180297-03-4P
180297-04-5P 180297-05-6P 180297-06-7P 180297-07-8P 180297-08-9P
180297-09-0P 180297-10-3P 180297-11-4P 180297-12-5P 180297-13-6P
RL: SPN (Synthetic preparation); PREP (Preparation)

(solid-phase synthesis of dialkylquinazolinediones)

L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:676982 CAPLUS
DN 123:286659
ED Entered STN: 14 Jul 1995
TI Liquid-phase combinatorial synthesis
AU Han, Hyunsoo; Wolfe, Mary M.; Brenner, Sydney; Janda, Kim D.
CS Dep. Mol. Biol. Chem., Scripps Res. Inst., La Jolla, CA, 92037, USA
SO Proceedings of the National Academy of Sciences of the United States of
America (1995), 92(14), 6419-23
CODEN: PNASA6; ISSN: 0027-8424
PB National Academy of Sciences
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 15, 25

AB A concept termed liquid-phase combinatorial synthesis (LPCS) is described.
The central feature of this methodol. is that it combines the advantages
that classic organic synthesis in solution offers with those that solid-phase
synthesis can provide, through the application of a linear homogeneous
polymer. To validate this concept two libraries were prepared, one of
peptide and the second of nonpeptide origin. The peptide-based library
was synthesized by a recursive deconvolution strategy (E. Erb, et al.,
1994), and several ligands found in this library bind a monoclonal
antibody elicited against β -endorphin. The non-peptide mols. were
arylsulfonamides, a class of compds. of known clin. bactericidal efficacy.
The results indicate that the reaction scope of LPCS should be general,
and its value to multiple, high-throughput screening assays could be of
particular merit, since multi-milligram quantities of each library member
can readily be attained.

ST liq phase combinatorial synthesis peptide; arylsulfonamide liq phase
combinatorial synthesis; **Merrifield synthesis**
polyethylene glycol support

IT Combinatorial library
Merrifield synthesis
(liquid-phase combinatorial synthesis of peptides and arylsulfonamides)

IT Peptides, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)

(mixts.; liquid-phase combinatorial synthesis of peptides and arylsulfonamides)

IT 56-40-6DP, Glycine, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 60-18-4DP, Tyrosine, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 61-90-5DP, Leucine, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 63-91-2DP, Phenylalanine, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 673-08-5DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 1050-28-8DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 17355-10-1DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 17355-11-2DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 21778-69-8DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 21778-72-3DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 21800-57-7DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 21841-54-3DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 60254-82-2DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 80638-46-6DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 111790-77-3DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 169692-75-5DP, pentapeptide polyethylene glycol monomethyl ether esters containing C-terminal 169692-76-6P 169692-77-7P 169692-78-8P 169692-79-9P 169692-86-8DP, disulfide conjugate with bovine serum albumin

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(liquid-phase combinatorial synthesis of peptides and arylsulfonamides)

IT 4530-20-5 6752-38-1, 4-(Chlorosulfonyl)**phenyl isocyanate** 9004-74-4 13139-15-6 13734-34-4 47689-67-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(liquid-phase combinatorial synthesis of peptides and arylsulfonamides)

IT 71921-24-9P 169692-80-2P 169692-81-3P 169692-82-4P 169692-84-6P 169692-87-9P 169692-88-0DP, alkylsulfonamide derivs.

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(liquid-phase combinatorial synthesis of peptides and arylsulfonamides)

IT 63-74-1DP, 4-Aminobenzenesulfonamide, alkylsulfonamide derivs. 169692-88-0P 169692-89-1P 169692-90-4P 169692-91-5P 169692-92-6P 169692-93-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(liquid-phase combinatorial synthesis of peptides and arylsulfonamides)

=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

40.41

40.62

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Dec 8, 2006 (20061208/UP).

=> s merrifield (W) synthesis and Phenyl(s) isothiocyanate

0 MERRIFIELD
13 SYNTHESIS
1 SYNTHESSES
13 SYNTHESIS
(SYNTHESIS OR SYNTHESSES)

0 MERRIFIELD (W) SYNTHESIS
0 PHENYL
0 ISOTHIOCYANATE
0 PHENYL(S) ISOTHIOCYANATE
L5 0 MERRIFIELD (W) SYNTHESIS AND PHENYL(S) ISOTHIOCYANATE

=> s merrifield (w) synthesis

0 MERRIFIELD
13 SYNTHESIS
1 SYNTHESSES
13 SYNTHESIS
(SYNTHESIS OR SYNTHESSES)

L6 0 MERRIFIELD (W) SYNTHESIS

=> file medline biosis caplus embase

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.24	40.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.75

FILE 'MEDLINE' ENTERED AT 11:29:26 ON 18 DEC 2006

FILE 'BIOSIS' ENTERED AT 11:29:26 ON 18 DEC 2006

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FILE 'EMBASE' ENTERED AT 11:29:26 ON 18 DEC 2006

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=> s merrifield (w) synthesis

L7 2983 MERRIFIELD (W) SYNTHESIS

=> s l7 and elman(w) degradation

L8 0 L7 AND ELMAN(W) DEGRADATION

=> s elman (w) degradation

L9 2 ELMAN (W) DEGRADATION

=> d 1-2 all

L9 ANSWER 1 OF 2 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN

AN 2002:529905 BIOSIS

DN PREV200200529905

TI The synthesis of a conformationally locked aminonucleoside analogue of the antibiotic puromycin.

AU Choi, Yongseok [Reprint author]; Strazewski, Peter; Marquez, Victor E.
[Reprint author]

CS Laboratory of Medicinal Chemistry, Center for Cancer Research, National
Cancer Institute at Frederick, Frederick, MD, 21702-1201, USA
yschoi@helix.nih.gov

SO Abstracts of Papers American Chemical Society, (2002) Vol. 223, No. 1-2,

pp. ORGN 217. print.

Meeting Info.: 223rd National Meeting of the American Chemical Society.
Orlando, FL, USA. April 07-11, 2002.

CODEN: ACSRAL. ISSN: 0065-7727.

DT Conference; (Meeting)
Conference; Abstract; (Meeting Abstract)
LA English
ED Entered STN: 16 Oct 2002
Last Updated on STN: 16 Oct 2002
CC General biology - Symposia, transactions and proceedings 00520
Pathology - Therapy 12512
Pharmacology - General 22002
Neoplasms - Therapeutic agents and therapy 24008
Chemotherapy - General, methods and metabolism 38502
Chemotherapy - Antiparasitic agents 38510
IT Major Concepts
Methods and Techniques; Pharmacology
IT Chemicals & Biochemicals
puromycin: antiinfective-drug, antineoplastic-drug, antiparasitic-drug,
antiprotozoal-drug, enzyme inhibitor-drug, analogs
IT Methods & Equipment
Elman degradation: synthetic method; Mitsunobu
reaction: synthetic method
IT Miscellaneous Descriptors
drug development; Meeting Abstract
RN 53-79-2 (puromycin)

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2002:190752 CAPLUS
ED Entered STN: 17 Mar 2002
TI The synthesis of a conformationally locked aminonucleoside analogue of the
antibiotic puromycin
AU Choi, Yongseok; Strazewski, Peter; Marquez, Victor E.
CS Laboratory of Medicinal Chemistry, Center for Cancer Research, Frederick,
MD, 21702-1201, USA
SO Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United
States, April 7-11, 2002 (2002), ORGN-217 Publisher: American Chemical
Society, Washington, D. C.
CODEN: 69CKQP
DT Conference; Meeting Abstract
LA English
AB The aminonucleoside produced by **Elman degrdn.** of the
antibiotic puromycin 1a exhibits trypanocidal as well as antitumor
properties (Figure 1). In 1972, Vince and Daluge synthesized a
carbocyclic cyclopentyl analog 2 lacking the 5'-OH group to avoid
formation of a nephrotoxic aminonucleotides that is normally produced from
puromycin. Since bicyclo[3.1.0]hexane nucleosides with a locked North
conformation are resistant to the action of cellular kinases, we
considered the synthesis of 3 as a 2'-deoxyribo version of aminonucleoside
analog 1b. One attractive feature of the target compound 3 is that by
virtue of its locked North conformation, the orientation of the critical
3'-NH2 would be conformationally equivalent to that found in the parent
aminonucleoside. In this work, the synthesis of a conformationally locked
carbocyclic aminonucleoside analog of the antibiotic puromycin will be
reported. Here, a 3-azido-substituted carbocyclic analog was coupled with
6-chloropurine under Mitsunobu conditions without concomitant reduction of an
azido group in the presence of tri-Ph phosphine.

=> s elman (w) method

L10 1 ELMAN (W) METHOD

=> d

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1969:104510 CAPLUS
DN 70:104510
TI Blood cholinesterase activity in acute and chronic hepatopathy
AU Terzani, Giuliano; Natalizi, Giorgio; Marinucci, Giovanni
CS Osp. Riuniti Roma, Rome, Italy
SO Laboratorio nella Diagnosi Medica (1968), 13(4-5), 139-51
CODEN: LDMEAC; ISSN: 0455-1222
DT Journal
LA Italian

=> s elman (w) degradation and phenyl (w) isothiocyanate
L11 0 ELMAN (W) DEGRADATION AND PHENYL (W) ISOTHIOCYANATE

=> s phenyl (w) isothiocyanate or PITC
L12 5251 PHENYL (W) ISOTHIOCYANATE OR PITC

=> s l12 and phenyl (w) isocyanate or PIC
L13 13030 L12 AND PHENYL (W) ISOCYANATE OR PIC

=> l13 and merrifield (w) synthesis
L13 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s l13 and merrifield (w) synthesis
L14 1 L13 AND MERRIFIELD (W) SYNTHESIS

=> d all

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:169538 CAPLUS
DN 118:169538
ED Entered STN: 01 May 1993
TI 9-Phenylxanthen-9-yl- (Pixyl): a new thiol protecting group and its use
in solid phase peptide chemistry
AU Echner, Hartmut; Voelter, Wolfgang
CS Physiol.-Chem. Inst., Univ. Tuebingen, Tuebingen, D-7400, Germany
SO Innovation Perspect. Solid Phase Synth. Collect. Pap., Int. Symp., 2nd
(1992), Meeting Date 1991, 371-5. Editor(s): Epton, Roger. Publisher:
Intercept, Andover, UK.
CODEN: 58OLAK
DT Conference
LA English
CC 34-1 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 27
AB A report from a symposium. Pixyl-substituted cysteine, which can be
easily prepared without serious side reactions, is stable under
9-fluorenylmethoxycarbonyl (Fmoc) solid-phase peptide coupling conditions.
Thus, condensation of 9-hydroxy-9-phenylxanthene (Pix-OH) with
cysteine in AcOH in the presence of BF3.OEt2 gave 87% H-Cys(Pix
) -OH, which was converted into the corresponding Fmoc derivative for
solid-phase syntheses. The new Pix protecting group is
removable with acids, iodine, mercury ions, and thallium compds. under
mild conditions.
ST phenylxanthanyl protective group cysteine symposium; **Merrifield**
synthesis phenylxanthanyl cysteine protection
IT **Merrifield synthesis**
(of cysteine-containing peptides, phenylxanthanyl side chain protection in)
IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(cysteine-containing, preparation of, by solid-phase methods,
phenylxanthanyl

side chain protection in)

IT Protective groups
 (phenylxanthenyl, for cysteine side chain in solid-phase peptide coupling reactions)

IT 596-38-3, 9-Hydroxy-9-phenylxanthene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation of, with cysteine side chain, boron trifluoride-promoted)

IT 146797-27-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and fluorenylmethoxycarbonylation of)

IT 146797-28-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and solid-phase peptide coupling reactions of)

IT 52-90-4, Cysteine, miscellaneous
 RL: MSC (Miscellaneous)
 (side chain protection of, with hydroxy(phenyl)xanthene, boron trifluoride-promoted)

=>

=> s Crk (w) II and FRET or fluorscence (w) resonance (w) energy (w) transfer
L15 3 CRK (W) II AND FRET OR FLUORSCENCE (W) RESONANCE (W) ENERGY (W)
TRANSFER

=> d3

D3 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter

"HELP COMMANDS" at an arrow prompt (=>).

=> d 1-3 all

L15 ANSWER 1 OF 3 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN
AN 2002:353776 BIOSIS

DN PREV200200353776

TI Determination of the capacity of TNF receptor associated factor (TRAF)-2
to form hetero- and homo-dimers by **fluorscence resonance**
energy transfer.

AU He, Liusheng [Reprint author]; Grammer, Amrie C.; Lipsky, Peter E.

CS Autoimmunity Branch, NIAMS, NIH, 9000 Rockville Pike, Bldg10, Rm6D48,
Bethesda, MD, 20892, USA

SO FASEB Journal, (March 20, 2002) Vol. 16, No. 4, pp. A314. print.

Meeting Info.: Annual Meeting of the Professional Research Scientists on
Experimental Biology. New Orleans, Louisiana, USA. April 20-24, 2002.
CODEN: FAJOEC. ISSN: 0892-6638.

DT Conference; (Meeting)

Conference; Abstract; (Meeting Abstract)

LA English

ED Entered STN: 26 Jun 2002

Last Updated on STN: 26 Jun 2002

AB The tumor necrosis factor receptor-associated factor (TRAF) family
proteins are cytoplasmic adaptor proteins that mediate signaling by a
variety of TNF receptor family members. Currently six members of this
family have been described. Besides the potential of TRAF family members
to form homotrimers, domains located in the C-terminal region of all TRAFs
potentially could mediate heterodimer formation with TRAF family members.
To date this possibility has been examined by in vitro immunoprecipitation
assays and GST fusion protein pull-down assays as well as yeast two hybrid
analysis. The capacity of homo- and heterodimerization has not been
examined thoroughly in living cells. To examine this, we employed an
approach using fluorescence energy transfer (FRET) which only occurs when
molecules are within 10-100 Angstroms. Constructs were produced
consisting of TRAF family members fused to yellow fluorescent protein
(YFP) or cyan fluorescent protein (CFP). YFP and CFP function as
appropriate donor and acceptor molecules for FRET. Using this approach,
we confirmed that TRAF2 interacts with itself and also with TRAF1 as
previously reported. Notably, however, TRAF2 had an interaction with
TRAF3 but not TRAFs 5 or 6, even though TRAF2 and TRAF5 colocalize to some
degree. These data provide more information on the potential role of TRAF
interactions in regulating the outcome of TNF receptor family signaling.

CC General biology - Symposia, transactions and proceedings 00520
Biochemistry studies - General 10060

IT Major Concepts

Biochemistry and Molecular Biophysics

IT Chemicals & Biochemicals

TNF receptor associated factor-2: heterodimerization, homodimerization;
cyan fluorescent protein; yellow fluorescent protein

IT Methods & Equipment

fluorescence resonance energy transfer: analytical method

IT Miscellaneous Descriptors

Meeting Abstract

L15 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:170631 CAPLUS
 DN 144:249410
 ED Entered STN: 24 Feb 2006
 TI **FRET** assay for c-Abl phosphorylation of **Crk-II**
 adapter protein utilizing semisynthetic dual-labeled proximity sensor
 peptide-containing **Crk-II** construct, and potential
 screening use
 IN Muir, Tom; Cotton, Graham
 PA USA
 SO U.S. Pat. Appl. Publ., 19 pp., Cont. of U.S. Ser. No. 483,543, abandoned.
 CODEN: USXXCO
 DT Patent
 LA English
 INCL 435007100
 CC 7-1 (Enzymes)
 Section cross-reference(s): 1, 34

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2006040319	A1	20060223	US 2004-784721	20040223
PRAI	US 2000-483543	B1	20000114		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2006040319	INCL	435007100
	IPCI	G01N0033-53 [I,A]
	IPCR	G01N0033-53 [I,A]; G01N0033-53 [I,C]
	NCL	435/007.100
	ECLA	C12Q001/48B; G01N033/542

AB Comps. and methods are provided for identifying conformational changes in polypeptides related to the activity or biol. state of the polypeptide. Semisynthetic polypeptides are prepared comprising at least two proximity-sensor peptides, the resultant composition capable of detectably indicating the activity of biol. state of the polypeptide. Such comps. may be used to identify modulators of the polypeptides as well as modulators of mols. which interact with the polypeptide, such as protein kinases which act on protein kinase targets. More specifically, the invention provides a biosensor for c-Abl phosphorylation of the **Crk-II** adapter protein. The structure of a dual-labeled, semisynthetic, recombinantly prepared composition comprising the protein kinase adapter protein **Crk-II** which is capable of reporting phosphorylation by c-Abl is disclosed. Generation of Rh-(**Crk-II**)-Fl (Rh = tetramethylrhodamine; Fl = fluorescein) by solid-phase protein ligation and phosphorylation of Rh-(**Crk-II**)-Fl by full-length c-Abl is reported. It was shown that Rh-(**Crk-II**)-Fl is a fluorescence biosensor for c-Abl phosphorylation of **Crk-II** utilizing **FRET** for c-Abl determination One potential use of this biosensor is in the rapid screening of c-Abl kinase inhibitors.

ST fluorescence biosensor cAbl kinase detn CrkII phosphorylation **FRET**
 ; proximity sensor peptide fluorescence biosensor protein kinase detn
 screening; **FRET** pair tetramethylrhodamine fluorescein proximity
 sensor peptide fluorescence biosensor

IT Proteins

RL: ARG (Analytical reagent use); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)

(CRKII, fusion products; **FRET** assay for c-Abl phosphorylation of **Crk-II** adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing **Crk-II** construct, and potential screening use)

IT Mus musculus

- (*Crk-II* of; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Dephosphorylation, biological
Drug screening
Fluorescent indicators
Phosphorylation, biological
Protein engineering
(*FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Enzymes, analysis
RL: ANT (Analyte); ANST (Analytical study)
(*FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Protein motifs
(SH2 domain; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Protein motifs
(SH3 domain; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Conformational transition
(activity-related, detection of; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Phosphorylation
(enzymic; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Fluorescence resonance energy transfer
(fluorescent label pair for; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Protein sequences
(of *Crk-II* construct; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Post-translational processing
(of peptide substrate; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Biosensors
(optical; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)
- IT Solid phase synthesis
(peptide, solid-phase protein ligation; *FRET* assay for c-Abl phosphorylation of *Crk-II* adapter protein utilizing semisynthetic dual-labeled proximity sensor peptide-containing *Crk-II* construct, and potential screening use)

IT Amino acids, uses
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (proximity sensor peptide containing fluorescent amino acid derivative;
FRET assay for c-Abl phosphorylation of **Crk-II** adapter protein utilizing semisynthetic dual-labeled
 proximity sensor peptide-containing **Crk-II** construct,
 and potential screening use)

IT Oligopeptides
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
 (Analytical study); PREP (Preparation); USES (Uses)
 (proximity sensor; **FRET** assay for c-Abl phosphorylation of
Crk-II adapter protein utilizing semisynthetic
 dual-labeled proximity sensor peptide-containing **Crk-II**
 construct, and potential screening use)

IT Proteins
 RL: ARG (Analytical reagent use); BPN (Biosynthetic preparation); ANST
 (Analytical study); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (recombinant, substrates; **FRET** assay for c-Abl
 phosphorylation of **Crk-II** adapter protein utilizing
 semisynthetic dual-labeled proximity sensor peptide-containing **Crk**
-II construct, and potential screening use)

IT Peptides, uses
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (substrate; **FRET** assay for c-Abl phosphorylation of
Crk-II adapter protein utilizing semisynthetic
 dual-labeled proximity sensor peptide-containing **Crk-II**
 construct, and potential screening use)

IT Phycoerythrins
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (β -, fluorescent label for **FRET**; **FRET** assay
 for c-Abl phosphorylation of **Crk-II** adapter protein
 utilizing semisynthetic dual-labeled proximity sensor peptide-containing
Crk-II construct, and potential screening use)

IT 146368-14-1, Cy5
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (Cy5, fluorescent label for **FRET**; **FRET** assay for
 c-Abl phosphorylation of **Crk-II** adapter protein
 utilizing semisynthetic dual-labeled proximity sensor peptide-containing
Crk-II construct, and potential screening use)

IT 9031-44-1, Kinase (phosphorylating) 98037-52-6, Abelson protein tyrosine
 kinase 138238-67-2, c-Abl kinase
 RL: ANT (Analyte); ANST (Analytical study)
 (**FRET** assay for c-Abl phosphorylation of **Crk-**
II adapter protein utilizing semisynthetic dual-labeled
 proximity sensor peptide-containing **Crk-II** construct,
 and potential screening use)

IT 876799-69-8P 876799-70-1P
 RL: ARG (Analytical reagent use); BPN (Biosynthetic preparation); BSU
 (Biological study, unclassified); PRP (Properties); SPN (Synthetic
 preparation); ANST (Analytical study); BIOL (Biological study); PREP
 (Preparation); USES (Uses)
 (amino acid sequence; **FRET** assay for c-Abl phosphorylation of
Crk-II adapter protein utilizing semisynthetic
 dual-labeled proximity sensor peptide-containing **Crk-II**
 construct, and potential screening use)

IT 91-64-5, Coumarin 129-00-0, Pyrene, uses 2321-07-5, Fluorescein
 6268-49-1, DABCYL 36930-63-9, IAEDANS 50402-56-7, EDANS 70281-37-7,
 Tetramethylrhodamine 138026-71-8, BODIPY 165599-63-3, BODIPY FL
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (fluorescent label for **FRET**; **FRET** assay for c-Abl
 phosphorylation of **Crk-II** adapter protein utilizing
 semisynthetic dual-labeled proximity sensor peptide-containing **Crk**
-II construct, and potential screening use)

1 FILES SEARCHED...

L16 1 EDMAN (W) DEGRADATION AND PITC AND PIC

=> d

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:331185 CAPLUS
DN 139:19286
TI An improved method for rapid sequencing of support-bound peptides by partial **edman degradation** and mass spectrometry
AU Sweeney, Michael C.; Pei, Dehua
CS Department of Chemistry and Ohio State Biochemistry Program, Ohio State University, Columbus, OH, 43210, USA
SO Journal of Combinatorial Chemistry (2003), 5(3), 218-222
CODEN: JCCHFF; ISSN: 1520-4766
PB American Chemical Society
DT Journal
LA English
RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE.FORMAT

=> s merrifield (w) synthesis and edman(w) degradation

L17 32 MERRIFIELD (W) SYNTHESIS AND EDMAN(W) DEGRADATION

=> d 25-32 abs

L17 ANSWER 25 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN
AB The **Edman degrdn.** was applied to the total sequence anal. of long peptides prepared by the solid-phase method in order to evaluate whether the reported min. level of preview in the anal. of omission in solid-phase peptide synthesis by **Edman degrdn.** was a real measure of synthetic efficiency or an artifact of the **Edman degrdn.**

L17 ANSWER 26 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN
AB The title study was discussed in terms of an anal. of a peptidyl resin in which the repetitive yield during degradation would be high and an anal. of a method to quantitate all of the amino acid phenylthiohydantoins encountered in the degradation of peptidyl resins.

L17 ANSWER 27 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN
AB H-Ala- [3H] Pro-Ala-Gly-Phe-Ala-Gly-Pam(AcAbu)-resin [Pam(AcAbu)-resin = hydroxymethylphenylacetamidomethyl(N-acetyl- α -aminobutramidomethyl)-resin] was prepared and then sequenced by the title degradation An average of 92% of the 1st 4 residues were removed from the peptidyl resin. Phenylthiohydantoins of side-chain protected amino acids were prepared and then characterized by high-pressure liquid chromatog. The 2-118 sequence of heavy-chain variable region of a homogeneous rabbit antibody was prepared by the solid-phase method, and the 117-residue peptidyl resin possessed the desired amino acid sequence according to a series of solid-phase **Edman degrdn.** expts.

L17 ANSWER 28 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN
AB The reaction of free N-terminal prolyl-peptides with isatin in the presence of BOC-Phe-OH to give a blue complex on the resin beads provides a rapid, sensitive, and selective test for the prolyl peptides. The accuracy of the test was similar to that of the 1st cycle of an **Edman degrdn.**

L17 ANSWER 29 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN
AB The 31-residue β -endorphin was prepared in 10% overall yield on a solid support of an amorphous copolymer of Me2C:CHCONH2, N,N'-

bisacryloylethylenediamine, and N-acryloyl-N'-tert-butoxycarbonyl- β -alanylhexamethylenediamine (10 days). The assembly of the polypeptide chain was monitored by solid-phase **Edman degrdn.**

L17 ANSWER 30 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB Ddz-Arg(NO₂)-Leu-Gln(Mbh)-Arg(NO₂)-Leu-Leu-Gln(Mbh)-Gly-Leu-Val-NHR (Ddz = α,α -dimethyl-3,5-dimethoxybenzyloxycarbonyl, Mbh = 4,4'-dimethoxybenzhydryl, R = benzhydrylpolystyrene resin) was prepared by the redox condensation method. **Edman degrdn.** of the peptide showed it to be 96% homogeneous.

L17 ANSWER 31 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB Peptides were prepared by coupling of a highly polar compound with the terminal NH₂ group of the desired sequence assembled on a solid support. Lysine was used as the highly polar compound. All protecting groups labile towards HF were removed as usual and the resulting crude peptide was purified through a carboxymethyl cellulose column. The terminal lysine residue was removed by **Edman degradation** to give the desired peptide. Thus, peptide fragments of the B chain of human insulin, H-Gly-Phe-Phe-Tyr-Thr-Pro-Lys-(Tfa)-Thr-OH and H-Gly-Ser-His-Leu-Val-OH, were prepared in good yield and in high purity.

L17 ANSWER 32 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB The Edman method of peptide degradation was modified. The peptides were bonded to the resin by a reverse **Merrifield synthesis** (CA 59: 7646b) and the degradation was carried out in the column. Thus, PTC-Ala-Phe-Gly (PTC = phenylthiocarbamoyl) (142.8 mg.) in 20 ml. absolute tetrahydrofuran was treated with 206 mg. dicyclohexylcarbodiimide and 2 g. aminomethylpolystyrene resin at -20°. The resin-bonded peptide thus obtained (500 g.) was treated with a mixture of 8 ml. H₂O and 12 ml. HCl-saturated AcOH at 40° to obtain PTH-Ala (PTH = 3-phenyl-2-thiohydantoin moiety). The resin was washed with saturated NaHCO₃, 5% Na₂CO₃, and water, treated dropwise with 50 ml. AcOH-Et₃N buffer and 50 ml. 1% PhCNS in Me₂CO, washed with C₆H₆, Me₂CO, and water and treated as above to release PTH-phenylalanine. PTH-Gly was released in the next cycle. The PTH-amino acids were identified by thin-layer chromatog. on silica gel (Kieselgel G) using 80:10 CHCl₃-MeOH (Pataki, CA 60: 12347a). The plates were sprayed with o-tolidine and exposed to Cl for 15 min. The R_f values were PTH-Ala 0.78, PTH-Phe 0.82, and PTH-Gly 0.67.

=> s merrifield (w) synthesis and edman(w) degradation and PITC and PIC

L18 0 MERRIFIELD (W) SYNTHESIS AND EDMAN(W) DEGRADATION AND PITC AND PIC

=> s merrifield (w) synthesis and edman(w) degradation and PITC

L19 0 MERRIFIELD (W) SYNTHESIS AND EDMAN(W) DEGRADATION AND PITC

=> d l17 20-25 all

L17 ANSWER 20 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1989:633585 CAPLUS

DN 111:233585

ED Entered STN: 23 Dec 1989

TI Solid-phase segment coupling: quality control by automated **Edman degradation** of peptidyl-resin

AU Van Rietschoten, J.; Sabatier, J. M.; Paroutaud, P.; Albericio, F.; Grandas, A.; Pedroso, E.; Giralt, E.

CS Lab. Biochim., Fac. Med., Marseille, 13326, Fr.

SO Colloque INSERM (1989), 174(Forum Pept., 2nd, 1988), 215-19
CODEN: CINMDE; ISSN: 0768-3154

DT Journal

LA English

CC 34-3 (Amino Acids, Peptides, and Proteins)

AB A report from a forum on peptides. Automated sequencing of peptides on a resin during solid-phase segment coupling is a useful and sensitive test for determining the yield of coupling of the segments.

ST **Merrifield synthesis** peptide Edman symposium;
Edman degrdn peptide resin symposium

IT **Merrifield synthesis**
(of peptides by segment coupling, automated **Edman degrdn.** of peptidyl resin as quality control test for)

IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by solid-phase segment method, automated **Edman degrdn.** of peptidyl resin as quality control test for)

IT **Edman degradation**
(automated, of peptide segments during solid-phase peptide synthesis)

L17 ANSWER 21 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1989:95782 CAPLUS

DN 110:95782

ED Entered STN: 17 Mar 1989

TI Solid phase synthesis and characterization of two canine gut gastrin-releasing peptides

AU De L. Milton, R. C.; Mayer, E.; Walsh, J. H.; Rivier, J. E.; Dykert, J.; Lee, T. D.; Shively, J. E.; Reeve, J. R., Jr.

CS Pept. Biol. Lab., Salk Inst., La Jolla, CA, USA

SO International Journal of Peptide & Protein Research (1988), 32(2), 141-52
CODEN: IJPPC3; ISSN: 0367-8377

DT Journal

LA English

CC 34-3 (Amino Acids, Peptides, and Proteins)

AB Two canine gastrin-releasing peptides, originally isolated from gut tissue exts., have been synthesized by solid phase methodol. and purified by preparative reverse phase high performance liquid chromatog. (RP-HPLC). The synthetic gastrin-releasing peptides GRP 1-27 and GRP 5-27 were characterized with regard to homogeneity and composition using nine different RP-HPLC systems, mass spectroscopy, amino acid anal., **Edman degrdn.**, methionine oxidation, and peptide mapping with tryptic, Staph. aureus V8 protease, and cyanogen bromide cleavage (the latter two systems performed only with GRP 1-27. Although a scarcity of the natural products prevented quant. biol. comparison of the synthetic and natural peptides, they elute identically on RP-HPLC chromatog., and similar dose dependent biol. potencies were observed in canine antral muscle tissue contraction expts. Indeed, all the peptides containing the bombesin-like carboxyl terminal decapeptide sequence studied to date have similar biol. activities.

ST gastrin releasing peptide **Merrifield synthesis**

IT 97730-71-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methionine oxidation of, with hydrogen peroxide)

IT 119221-10-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 97730-72-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by solid-phase method)

IT 2488-15-5, N-tert-Butoxycarbonylmethionine 4530-20-5,
N-tert-Butoxycarbonylglycine 7536-58-5 13139-14-5 13139-15-6
13734-41-3 13836-37-8 15260-10-3 15761-38-3, N-tert-
Butoxycarbonylalanine 15761-39-4 23680-31-1 35899-43-5 40298-71-3
54613-99-9 55260-24-7 65420-40-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase peptide coupling reactions of)

L17 ANSWER 22 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1985:145646 CAPLUS
 DN 102:145646
 ED Entered STN: 04 May 1985
 TI Synthesis of side chain-protected amino acid phenylthiohydantoins and their use in quantitative solid-phase **Edman degradation**
 AU Steiman, David M.; Ridge, Richard J.; Matsueda, Gary R.
 CS Harvard Med. Sch., Boston, MA, 02114, USA
 SO Analytical Biochemistry (1985), 145(1), 91-5
 CODEN: ANBCA2; ISSN: 0003-2697
 DT Journal
 LA English
 CC 9-10 (Biochemical Methods)
 Section cross-reference(s): 34
 AB Solid-phase **Edman degrdn.** of synthetic peptidyl-resins was used advantageously to detect errors of deletion which might occur during Merrifield peptide synthesis. To facilitate complete quantitation of the resulting phenylthiohydantoin(PTH)-amino acids, the PTH derivs. of the following side chain-protected amino acid residues have been synthesized: Arg(Tos), Asp(OBzl), Cys(3,4-(CH₃)₂-Bzl), Glu(OBzl), Lys(2-ClZ), Ser(Bzl), Thr(Bzl), Tyr(2-BrZ), and Tyr(2,6-Cl₂Bzl). Tos is tosyl-(p-toluenesulfonyl-), OBzl is o-benzyl, and -Clz is chlorobenzoyloxycarbonyl. For each derivative, a m.p., elemental anal., and absorptivity were obtained. With these new compds. as HPLC stds., an unequivocal assignment and quantification of each side chain protected amino acid was possible. A quant. anal. was performed for 6 model peptides with the general formula Ala-X-Leu-Y-Ala-Gly-NHCH₂-resin (where X and Y represented different side chain-protected amino acyl residues). Solid-phase **Edman degrdn.** was a useful aid for the characterization of peptides when they are used unpurified as synthetic antigens.
 ST protected amino acid phenylthiohydantoin prepn; **Edman degrdn** peptide prepn Merrifield; HPLC amino acid phenylthiohydantoin
 IT **Merrifield synthesis**
 (of peptides, errors of deletion in, detection of, solid-phase **Edman degrdn.** of synthetic peptidyl-resins for)
 IT Melting point
 Molecular weight
 (of side chain-protected amino acid phenylthiohydantoins)
 IT Peptides, preparation
 RL: PREP (Preparation)
 (preparation of, by **Merrifield synthesis**, errors of deletion in, detection of)
 IT Chromatography, column and liquid
 (high-performance, of side chain-protected amino acid phenylthiohydantoins)
 IT Absorptivity
 (molar, of side chain-protected amino acid phenylthiohydantoins)
 IT **Edman degradation**
 (solid-phase, of synthetic peptidyl-resins, for detecting errors of deletion in Merrifield peptide synthesis)
 IT 68-12-2, uses and miscellaneous
 RL: USES (Uses)
 (-diisopropylamine buffer, for solid-phase degradation)
 IT 108-18-9
 RL: ANST (Analytical study)
 (-dimethylformamide buffer, for solid-phase **Edman degrdn.**)
 IT 54613-99-9
 RL: ANST (Analytical study)
 (in side-chain-protected amino acids preparation)
 IT 66629-67-2P 66629-70-7P 66629-71-8P 66629-72-9P 76877-35-5P
 76877-36-6P 77876-58-5P 77876-59-6P 77876-61-0P 95759-19-6P
 95759-20-9P

RL: PREP (Preparation)

(preparation and characterization of)

IT 77876-53-ODP, resin bound 95759-21-ODP, resin bound

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and solid-phase *Edman degrdn.* of)

L17 ANSWER 23 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:192240 CAPLUS

DN 100:192240

ED Entered STN: 08 Jun 1984

TI Solid-phase synthesis of sauvagine-(17-40)

AU Santangelo, Francesco; Montecucchi, Pier Carlo; Gozzini, Luigia; Henschen,
Agnes

CS Chem. Res. Dep., Farmitalia Carlo Erba, S.p.A., Milan, Italy

SO International Journal of Peptide & Protein Research (1983), 22(3), 348-54
CODEN: IJPPC3; ISSN: 0367-8377

DT Journal

LA English

CC 34-3 (Amino Acids, Peptides, and Proteins)

GI

H-Met-Ile-Glu-Ile-Glu-Lys-Gln-Glu-

Lys-Glu-Lys-Gln-Gln-Ala-Ala-Asn-

Asn-Arg-Leu-Leu-Leu-Asp-Thr-Ile-NH₂ I

AB The title peptide (I) was prepared by the solid-phase method on a
benzhydrylamine resin. I was purified by gel filtration and had an
acceptable degree of homogeneity according to electrophoresis, chromatog.,
and automated *Edman degrdn.* anal. I was devoid of any
sauvagine activity on the circulatory system and endocrine glands, and it
exhibited a weak effect on gastric emptying delay.

ST sauvagine tetracosapeptide *Merrifield synthesis*

IT *Merrifield synthesis*

(of sauvagine sequence 17-40)

IT 74434-59-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of sequence 17-40 of, by solid-phase method)

IT 88831-26-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by solid-phase method)

L17 ANSWER 24 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:51962 CAPLUS

DN 100:51962

ED Entered STN: 12 May 1984

TI Synthesis of the protected tridecapeptide (56-68) of the VH domain of
mouse myeloma immunoglobulin M603 and its reattachment to resin supports

AU Voss, Christoph; Dimarchi, Richard; Whitney, Donald B.; Tjoeng, Foe Siong;
Merrifield, R. B.; Tam, James P.

CS Rockefeller Univ., New York, NY, 10021, USA

SO International Journal of Peptide & Protein Research (1983), 22(2), 204-13
CODEN: IJPPC3; ISSN: 0367-8377

DT Journal

LA English

CC 34-3 (Amino Acids, Peptides, and Proteins)

AB The title protected tridecapeptide was prepared by solid-phase peptide
synthesis using the photolabile 4-bromomethyl-3-nitrobenzamidomethyl-resin
and the multidetachable 2-[4-(bromomethyl)phenylacetoxy]propionyl-resin as
solid supports. The protected tridecapeptide was removed photolytically

from both supports and the sequence integrity was determined by preview anal. using the solid-phase **Edman degrdn.** procedure. The protected tridecapeptide was reattached to 4-bromomethyl-3-nitrobenzamidomethyl-resin to give the photolabile Boc-protected peptidyl 4-oxymethyl-3-nitrobenzamidomethyl-resin (Boc = Me₃CO₂C) in 25% yield. The protected tridecapeptide-oxymethylphenylacetic acid derivative was reattached to aminomethyl-resin to give Boc-protected peptidyl-2-[(4-oxymethyl)phenyl]acetamidomethyl-resin in 45% yield and to 2-bromopropionyl-resin generating the multidetachable Boc-protected peptidyl-2-[(4-oxymethyl)phenylacetoxyl]propionyl-resin in 80% yield. The reactivity of these reattached peptides was demonstrated by the quant. coupling of Boc-Leu-OH to the protected peptide-resin. The advantages and disadvantages of the different resins with respect to solid-phase fragment synthesis are discussed.

- ST myeloma Ig tridecapeptide **Merrifield synthesis**;
photolabile resin tridecapeptide; photolysis tridecapeptide resin
- IT **Merrifield synthesis**
(of tridecapeptide of VH domain of myeloma IgM603 on photolabile resins, reattachment to resin supports in relation to)
- IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, of myeloma IgM603 VH domain sequence, by solid-phase method on photolabile resins, reattachment to resin supports in relation to)
- IT 67521-49-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with bromopropionyl-resin)
- IT 88466-10-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and attachment of, to bromopropionyl-resin)
- IT 88466-09-5DP, ester with [(hydroxymethyl)phenyl]acetoxylpropionyl-resin
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and photolytic resin cleavage of)
- IT 4530-20-5DP, ester with [(hydroxymethyl)phenyl]acetoxylpropionyl-resin
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and solid-phase peptide synthesis with)
- IT 88480-64-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 13139-15-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase peptide coupling of)

L17 ANSWER 25 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1983:422893 CAPLUS

DN 99:22893

ED Entered STN: 12 May 1984

TI A study of the **Edman degradation** in the assessment of the purity of synthetic peptides

AU Kent, Stephen B. H.; Riemen, Mark; LeDoux, Marie; Merrifield, R. B.

CS Rockefeller Univ., New York, NY, 10021, USA

SO Methods Protein Sequence Anal., [Proc. Int. Conf.], 4th (1982), Meeting Date 1981, 205-13. Editor(s): Elzinga, Marshall. Publisher: Humana, Clifton, N. J.

CODEN: 49KBAY

DT Conference

LA English

CC 34-3 (Amino Acids, Peptides, and Proteins)

AB The **Edman degrdn.** was applied to the total sequence anal. of long peptides prepared by the solid-phase method in order to evaluate whether the reported min. level of preview in the anal. of omission in solid-phase peptide synthesis by **Edman degrdn.** was a real measure of synthetic efficiency or an artifact of the **Edman degrdn.**

ST **Edman degrdn** purity peptide; **Merrifield**

synthesis peptide Edman degrdn

IT **Edman degradation**
(of peptides prepared by solid-phase method)

IT Protein sequences
(of peptides prepared by solid-phase method, sequencing of, by **Edman degrdn.**)

IT **Merrifield synthesis**
(of peptides, sequencing by **Edman degrdn.** in relation to)

IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by solid-phase method, sequencing by **Edman degrdn.** in relation to)

IT 2010-15-3 4332-95-0 4332-97-2 4333-19-1 4333-20-4 4333-21-5
4370-90-5 4399-40-0 5066-94-4 5624-08-8 5835-68-7 79162-62-2
86124-51-8 86124-52-9 86124-53-0 86124-54-1 86124-55-2
86124-56-3 86124-57-4 86124-58-5 86124-59-6 86124-60-9
RL: PROC (Process)
(separation of, by reverse-phase high-performance liquid chromatog.)

IT 80451-04-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequencing of synthetic 1-33 fragment of, by **Edman degrdn.**)

IT 9035-22-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequencing of synthetic 135-155 fragment of, by **Edman degrdn.**)

IT 9061-61-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequencing of synthetic fragment of, by **Edman degrdn.**)

IT 86124-61-0 86124-62-1 86124-63-2 86124-64-3 86124-65-4
86124-66-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequencing of, by **Edman degrdn.**)

IT 61214-51-5 69521-94-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthetic, sequencing of, by **Edman degrdn.**)

=> d 1-5 abs

L19 HAS NO ANSWERS

'1-5 ' IS NOT A VALID SEARCH STATUS KEYWORD

Search status keywords:

NONE ---- Display only the number of postings.

STATUS -- Display statistics of the search.

ENTER SEARCH STATUS OPTION (NONE), STATUS, OR ?:none

L19 0 SEA MERRIFIELD (W) SYNTHESIS AND EDMAN(W) DEGRADATION AND PITC

=> d 117 1-5 abs

L17 ANSWER 1 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB ω -Agatoxin IVA, isolated from the venom of funnel web spider
Agelenopsis aperta, blocks potently and selectively P-type calcium channels. This toxin, composed of 48 amino acids and containing 8 Cys residues, was synthesized by the solid-phase procedure. The Cys residues were protected by acetamidomethyl (Acm) groups which were removed by mercuric acetate. During treatment with mercuric acetate, a byproduct was detected, involving modification of Trp residues by the Acm groups. This side reaction can be completely prevented by addition of an excess of Trp in the reaction medium during Acm deprotection. The resulting peptide was submitted to an oxidative refolding, in different conditions, in order to determine the most favorable protocol. After formation of the four disulfide

bonds, the toxin was purified by successive preparative HPLC, on two different supports, and fully characterized by anal. HPLC, capillary electrophoresis, amino acid anal., mass spectrometry and **Edman degrdn.** It was found to block the P-type calcium channel with a similar biol. potency as described for the natural product.

L17 ANSWER 2 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN
GI

FMOC-Ala-Phe-Val┐
FMOC-Ala-Phe-Val-Lys┐
 BOC-Gly-Tyr-Leu-Lys-SCAL-TG I

AB A library for identifying and analyzing ligands of acceptors of interest comprises: a multiplicity of solid supports to which are attached (1) a species of test compound comprised of a series of subunits, and (2) a species of coding mol. which is topol. segregated from the test compound; the sequence of subunits of the test compound attached to a particular support is encoded by the coding mol. attached to the same support. Each of the solid phase synthesis support beads contains a single type of synthetic test compound. The synthetic test compound can have backbone structures with linkages such as amide, urea, carbamate, ester, amino, sulfide, disulfide, or carbon-carbon, such as alkane and alkene, or any combination thereof. The synthetic test compound can also be a mol. scaffold, such as derivs. of monocyclic or bicyclic carbohydrates, steroids, sugars, heterocyclic structures, polyarom. structures, etc. The coding mol. (preferably a peptide) may be segregated in the interior of the support and the test compound on the exterior, accessible to a macromol. acceptor mol. of interest. Thus, BOC-Lys(FMOC)-OH was coupled to safety catch amide linker (SCAL)-modified tentagel (TG) resin; the Ne-FMOC group was removed and FMOC-Lys(FMOC)-OH was coupled to the side chain of the first Lys. The FMOC groups were removed and the resin was divided into 3 parts, which were sep. coupled with FMOC-Ala-OH, FMOC-Phe-OH, and FMOC-Val-OH. Corresponding (coding) amino acids BOC-Gly-OH, BOC-Tyr-OH, and BOC-Leu-OH were then coupled to the N α -position of Lys after BOC deprotection. Further division and peptide coupling steps gave a total of 27 tripeptide moieties such as (I), in which the FMOC-protected tripeptides represent the test compound and the BOC-protected tripeptide represents the coding mol. Replacement of the BOC protecting group with F3CCO was followed by sequencing of the coding peptide.

L17 ANSWER 3 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB Combinatorial libraries employing the one-bead-one-compound technique are reviewed with 122 refs.. Two distinguishing features characterize this technique. First, each compound is identified with a unique solid support, enabling facile segregation of active compds. Second, the identity of a compound on a pos. reacting bead is elucidated only after its biol. relevance is established. Direct methods of structure identification (**Edman degrdn.** and mass spectroscopy) as well as indirect "coding" methods facilitating the synthesis and screening of nonpeptide libraries are discussed. Nonpeptide and "scaffold" libraries, together with a new approach for the discovery of a peptide binding motif using a "library of libraries", are also discussed. In addition, the ability to use combinatorial libraries to optimize initially discovered leads is illustrated with examples using peptide libraries.

L17 ANSWER 4 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB Fast and convenient binding assays using synthetic peptides are of utmost and increasing importance, especially in the search for lead structures or in

the field of diagnostics. A polymeric support suitable for solid-phase peptide synthesis was functionalized with two different anchor groups. The interior part of the aminomethylated polystyrene-1%-divinylbenzene resin beads, comprising about 98% of the total loading capacity, was modified by the acid-labile 5-(2-aminomethyl-3,5-dimethoxyphenoxy)valeric acid (ADPV) anchor whereas the 2% outer surface of the polymer was covalently coated with a polyethylene glycol (PEG) 10,000 derivative which renders the resin surface hydrophilic and biocompatible. The novel resin was characterized by introducing marker amino acids and by IR. Employing this bifunctionalized resin for peptide synthesis, free as well as polymer-bound peptides were obtained which were tested for recognition by antibody. The resin-bound peptides proved to be suitable for ELISA and fluorescence assays, as shown by confocal laser microscopic investigations. Peptides from the interior part were obtained in high yield and purity as analyzed by HPLC, electrospray mass spectrometry and *Edman degrdn.*

L17 ANSWER 5 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB The current high-sensitivity mode of automated sequencing by *Edman degrdn.*, as applied to solid-phase peptide synthesis using the tert-butoxycarbonyl (Boc)/benzyl protection strategy, is described. Major characteristics of this method are described, with complications and limitations explained.

=> d 117 6-15 abs

L17 ANSWER 6 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

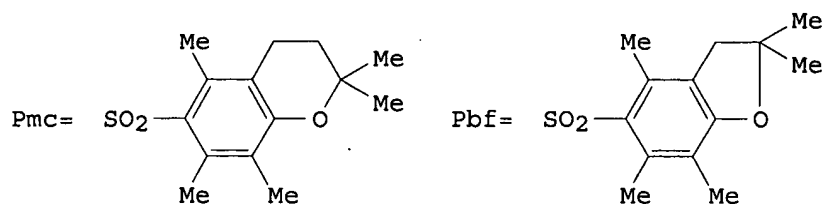
AB Assay conjugates comprising an active peptide/peptoid, an encoding polymer (DNA, RNA, or peptide/peptoid), and a coupling moiety covalently bonded to the active peptide and the encoding polymer, were prepared. Mixts. of potentially active diverse oligopeptides and/or peptide-like compds. may be synthesized along with an associated encoding polymer (a peptide/peptoid or a DNA strand). These conjugates may be screened for biol. activity and the active conjugates may be analyzed by, e.g., DNA sequencing methods to determine the attached peptide/peptoid sequence by deduction, i.e., since each DNA sequence is associated with a known peptide/peptoid, once the DNA sequence is determined, the sequence of the peptide/peptoid can be deduced. Q1-(MBHA resin)-Q2 [Q1 = Ac-Arg-Leu-Val-Thr-His, (binding sequence), Q2 = H-Ala-Ser-Gly-Glu-Phe-Ala, (coding sequence)] was prepared via alternate coupling of Fmoc-protected amino acids and Ddz-protected amino acids; a sequencing method using *Edman degrdn.* of the coding sequence was described. Another peptide-peptide conjugate using a nonpolymeric coupling moiety was prepared and its affinity for an anti-gp120 antibody was investigated; binding activity was unaffected by the coding peptide.

L17 ANSWER 7 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB The small protein ubiquitin (76 amino acids) has been synthesized under optimized conditions by Merrifield solid-phase methodol. using the N α -9-fluorenylmethoxycarbonyl (Fmoc) protecting group. The crude polypeptide mixture was purified to homogeneity by gel filtration, dialysis and a combination of cation- and anion-exchange chromatog. to yield ubiquitin. Amino acid anal., enzymic digestion and sequencing by automated *Edman degrdn.* were used to authenticate the primary structure. Isoelec. focusing and mass spectrometry were used to demonstrate that the final product was >98% pure with a final yield of 93 mg (4.3%) from a single synthesis on a 0.25 nmol scale.

L17 ANSWER 8 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

GI



AB This study examined Pmc and Pbf side-chain protection of Arg and Boc side-chain protection of Trp in an attempt to minimize side-chain protecting group "scavenger" use following Fmoc-based solid-phase synthesis. The extent of Trp alkylation was characterized and quantitated by anal. RP-HPLC, *Edman degrdn.* sequence anal., and ESMS. The Pbf group offered lower TFA-induced Trp alkylation than the Pmc group. The combination of Trp(Boc) and Arg(Pbf) resulted in extremely low levels of Trp alkylation during TFA treatment of the peptide-resin in the absence of scavengers.

L17 ANSWER 9 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB A generally applicable solid-phase methodol. has been developed for the synthesis of triple-helical polypeptides incorporating native collagen sequences. Three nascent peptide chains are C-terminal linked through one N α -amino and two N ϵ -amino groups of Lys, while repeating Gly-Pro-Hyp triplets induce triple helicity. Different protecting group strategies, including several three-dimensionally orthogonal schemes, have been utilized for the synthesis of four homotrimeric triple-helical polypeptides (THPs) of 79-124 residues, three of which incorporate native type IV collagen sequences. Highly efficient assemblies were achieved by 9-fluorenylmethoxycarbonyl (Fmoc) N α -amino group protection, in situ 2-(1H-benzotriazole-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate mediated couplings, and DBU-mediated Fmoc group removal. THPs were characterized by *Edman degrdn.* sequencing, size-exclusion chromatog., mass spectrometry, reversed-phase high performance liquid chromatog., and CD spectroscopy. THF thermal stabilities ranged from 35 to 59°, with chain length and Hyp content being the influential factors. Melting temps. and van't Hoff enthalpies for peptide triple-helical denaturation could be correlated well to Hyp content. The THP synthetic protocol developed here will allow for the study of both structure and biol. activity of specific collagen sequences in homotrimeric and heterotrimeric forms.

L17 ANSWER 10 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB A method of indirectly determining the structure of nonpeptide or nonsequenceable compds. that have been synthesized on individual particles of solid support is described. The technique permits the parallel synthesis of a compound that is not susceptible to *Edman degrdn.* (e.g., N-terminal-blocked peptide), or one containing components that cannot be identified by amino acid sequencing, together with a corresponding "coding" peptide. Each coupling step in the assembly of the nonsequenceable compound is followed by the coupling of an amino acid to a different attachment site of the same carrier particle, whereby the amino acid unambiguously codes for the previously coupled building block of the nonsequenceable compound. The rationale is to enable the sequence determination of a biol. active compound that has been identified through the screening of a library of nonsequenceable compds., by translating the sequence of its "coding" peptide, determined by *Edman degrdn.* .. into the structure of the active compound. The technique facilitates the construction and screening of nonpeptide libraries for the discovery of important pharmaceutical compds.

L17 ANSWER 11 OF 32 CAPLUS COPYRIGHT 2006 ACS on STN

AB The efficacy of *Edman degrdn.* sequence anal. for

evaluating the synthetic efficiency of peptide-resin assembly by 9-fluorenylmethoxycarbonyl (Fmoc) solid-phase methodol. has been studied. Prior researchers have described the use of solid-phase "preview" sequence anal. for peptides synthesized by tert-butyloxycarbonyl chemical, where benzyl-based side-chain protecting groups and peptide-resin linkers are stable to the conditions of Edman chemical. The authors have successfully sequenced a variety of resin-bound peptides synthesized by Fmoc chemical, where tert-butyl-based side-chain protecting groups and peptide-resin linkers are labile to the conditions of Edman chemical. Crude peptides are liberated from trifluoroacetic acid-labile linkers during the first cycle of *Edman degrdn.* and subsequently "embedded" in membranes. For peptides up to 20 residues, embedded sequencing repetitive yields were comparable to those of solid-phase sequencing. Preview sequencing of resin-bound Fmoc-synthesized peptides proved to be advantageous compared to other anal. methods, in that synthetic failures were detected and quantitated at the point of occurrence, regardless of whether incomplete Fmoc deprotection or incomplete coupling was responsible, and without interference from byproducts formed during peptide-resin cleavage. Quant. ninhydrin anal., which previously has been found to give false pos. results due to removal of the Fmoc group by a combination of reagents and high temperature, gave false neg. results in this study, most probably due to incomplete removal of the Fmoc group prior to coupling. Quant. sequence anal. results were supported by high-performance liquid chromatog., amino acid and electrospray mass spectrometric analyses of the crude and purified peptides.

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AB A peptide corresponding to the native 1-66 sequence of horse heart cytochrome c has been synthesized by stepwise automated solid-phase methods on PAM resin. The course of the synthesis has been monitored by several anal. methods including quant. ninhydrin and *Edman degrdn.* After HF cleavage, the peptide has been purified by a combination of semipreparative ion-exchange and RP-HPLC. The homogeneity of the purified synthetic peptide has been determined by different criteria including HPLC, amino acid composition, electrophoresis, antibody binding, tryptic and chymotryptic peptide mapping. After deprotection of the AcM-Cys residues and CNBr cleavage of the Met65-Glu66 peptide bond with simultaneous transformation of the Met65 residue into the activated C-terminal [Hse65]lactone, this purified synthetic peptide has been utilized for conformation-assisted joining expts. in combination with synthetic (66-104) to produce fully synthetic [Hse65]apocytochrome c. This latter, after mitochondria-mediated stereospecific heme insertion, has given a functional mol. corresponding to native horse heart holocytochrome c.

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AB Defensins are a group of small, cationic, antimicrobial proteins found in the cytoplasmic granules of neutrophils and macrophages of a variety of mammalian species. One such defensin, NP-1, isolated from rabbit neutrophils, consists of 33 amino acids rich in arginine and cysteine. Rabbit NP-1 was prepared on an Applied Biosystems Model 431A peptide synthesizer using FastMoc® chemical involving 2-1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate activation for coupling amino acids. The linear peptide was folded by air oxidation to the biol. active form containing three disulfide bonds and purified by reverse phase chromatog. The amino acid sequence of the synthetic peptide was confirmed by *Edman degrdn.* Mol. weight determination by plasma desorption mass spectrometry gave a value of 3898.6, in agreement with the expected mol. weight of 3898. The biol. activity of the synthetic peptide, as measured by its antifungal activity against several pathogenic fungi, was indistinguishable from that of the natural NP-1. Also, the CD was equivalent to that of natural NP-1, indicating conformational identity of the two species.

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AB The 36-amino-acid neuropeptide Y (human), which is one of the most potent vasoconstrictors and which exhibits a number of other biol. functions, has been synthesized using automated peptide synthesis. The optimized method, using 9-fluorenylmethoxycarbonyl protecting and single-step coupling, yielded the crude product in 90% purity allowing for single-step reversed-phase HPLC purification to >98% purity and a high overall yield (50%). The hormone was characterized by several chromatog. methods, ion-spray mass spectroscopy and *Edman degrdn.* The conformation of human neuropeptide Y was examined by CD, NMR and computer simulation. The CD measurements in trifluoroethanol/water (9:1) show a large percentage of α -helix. Variation of concentration from 0.5 μ M increasing up to the 1 mM used for NMR measurements, indicates no evidence for aggregation. In the same solvent system, the NMR line widths were very broad and therefore the resonance assignment was achieved with the exclusive use of 2-dimensional NOE spectra. The 248 clearly distinguishable NOEs from the NMR study were used in distance geometry calcns. and the resulting structures were refined with restrained mol. dynamics. The results indicate an α -helix extending from Arg19 to Gln34. For the N-terminal half of the mol. no regular structure was observed

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AB A rapid, high yielding, synthesis of endothelial interleukin-8 [Ala-IL8]77 has been achieved by automated solid phase peptide synthesis using an optimized protocol based on the tert-butoxycarbonyl (Boc)-benzyl combination, 2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium tetrafluoroborate (TBTU) activation and "in situ neutralization". Comparison with the synthesis of monocyte interleukin-8 [Ser-IL8]72 using the DCC/1-hydroxybenzotriazole (HOBt) activation method is made. Both syntheses gave 50-90 mg of pure product on 0.3-0.4 mmol initial loading in less than twelve working days. Rigorous quality control (amino acid anal., *Edman degrdn.*, HPLC, capillary zone electrophoresis, ion spray mass spectrometry) was used to assess the chemical integrity of the peptides.

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